

# Orbital-selective Mott transitions in two-band Hubbard models

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## Abstract

The anisotropic two-orbital Hubbard model is investigated at low temperatures using high-precision quantum Monte Carlo (QMC) simulations within dynamical mean-field theory (DMFT). We demonstrate that two distinct orbital-selective Mott transitions (OSMTs) occur for a bandwidth ratio of 2 even without spin-flip contributions to the Hund exchange, and we quantify numerical errors in earlier QMC data which had obscured the second transition. The limit of small inter-orbital coupling is introduced via a new generalized Hamiltonian and studied using QMC and Potthoff's self-energy functional method, yielding insight into the nature of the OSMTs and the non-Fermi-liquid OSM phase and opening the possibility for a new quantum-critical point.

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## 1. Introduction

Recently, the suggestion [1] that the two consecutive phase transitions experimentally observed [2] in  $\text{Ca}_{2-x}\text{Sr}_x\text{RuO}_4$  should be interpreted as “orbital-selective Mott transitions” (OSMTs) sparked a cascade of related theoretical papers (see [3] and references therein).

Microscopic studies of OSMTs usually consider the 2-band Hubbard model  $H = H_1 + H_2 + H_3$ , where

$$H_1 = - \sum_{\langle ij \rangle m \sigma} t_m c_{im\sigma}^\dagger c_{jm\sigma} + U \sum_{im} n_{im\uparrow} n_{im\downarrow},$$

$$H_2 = \sum_{i\sigma\sigma'} (U' - \delta_{\sigma\sigma'} J_z) n_{i1\sigma} n_{i2\sigma'}$$

include hopping between nearest-neighbor sites  $i, j$  with amplitude  $t_m$  for orbital  $m \in \{1, 2\}$ , *intra*- and *inter*-orbital Coulomb repulsion parametrized by  $U$  and  $U'$ , respectively, and Ising-type Hund's exchange coupling;  $n_{im\sigma} = c_{im\sigma}^\dagger c_{im\sigma}$  for spin  $\sigma \in \{\uparrow, \downarrow\}$ . In addition,

$$H_3 = \frac{1}{2} J_\perp \sum_{im\sigma} c_{im\sigma}^\dagger \left( c_{i\bar{m}\sigma}^\dagger c_{im\bar{\sigma}} + c_{im\sigma}^\dagger c_{i\bar{m}\bar{\sigma}} \right) c_{i\bar{m}\sigma}$$

contains spin-flip and pair-hopping terms (with  $\bar{1} \equiv 2, \bar{\uparrow} \equiv \downarrow$  etc.). As in [3], we refer to  $H_1 + H_2 + H_3$  with the isotropic coupling  $J_z = J_\perp \equiv J$  as the  $J$ -model and to the simplified

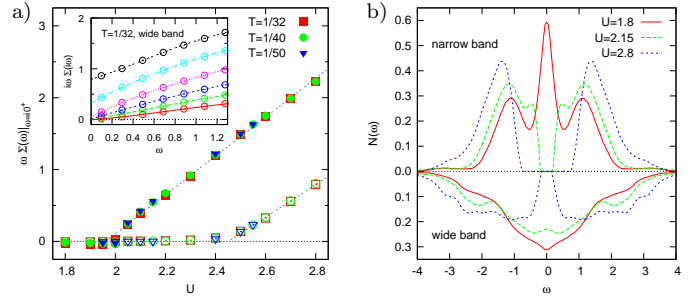


Fig. 1. a) Low-frequency analysis of self-energy. Main panel: weight of singularity at  $\omega = 0$  for narrow/wide band (filled/open symbols) as determined by polynomial fits [shown in inset for  $U = 2.8, 2.6, 2.4, 2.2, 2.0, 1.8$  (top to bottom)]. b) Spectra for metallic, orbital-selective, and insulating phases.

Hamiltonian  $H_1 + H_2$  as the  $J_z$ -model; unless noted,  $U' = U/2$ ,  $J = U/4$  so that  $U' + 2J = U$ .

Early theoretical studies suggested that the expected 2 distinct OSMTs occur only in the full  $J$  model [4], but not in the Ising type  $J_z$ -model [5,6]. Thus, it seemed as if spin-flip and pair-hopping terms were essential ingredients to orbital-selective physics. However, this is not actually the case, as shown in a low-frequency analysis of high-precision QMC data [3] in Fig. 1a: a singularity develops at  $\omega = 0$  for  $U_{c1} \approx 2.0$  in the narrow-band self-energy, but only at  $U_{c1} \approx 2.5$  in the wide-band self-energy (with linear increase for  $U > U_{c1/2}$ ). Corresponding spectra (Fig. 1b) illustrate the characteristics of the 3 distinct phases.

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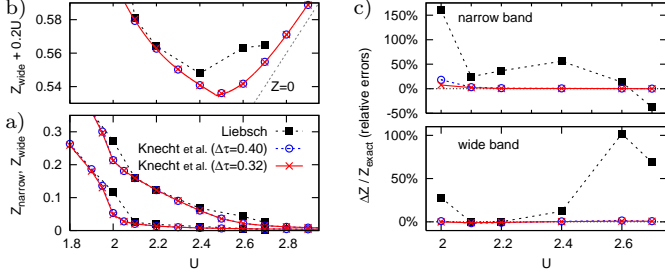


Fig. 2. a) QMC estimates of quasiparticle weights  $Z$  at  $T = 1/32$ : a) high-precision data [3] (circles, crosses) clearly shows kinks at  $U_{c1} \approx 2.0$ ; b) suitable analysis reveals a second kink at  $U_{c2} \approx 2.5$ . The second transition is lost in the noise of earlier data [5] (squares) with errors exceeding 100% at both transitions (c).

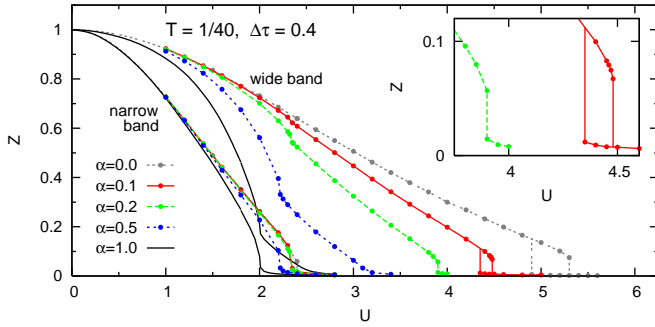


Fig. 3. Quasiparticle weights for generalized two-orbital model: at  $T = 1/40$ , the wide-band transition remains first order (with hysteresis) for small enough inter-orbital coupling  $\alpha \lesssim 0.2$ .

Discrete estimates  $Z = [1 - \text{Im} \Sigma(i\pi T)/(\pi T)]^{-1}$  for the quasiparticle weight clearly show (only) the narrow-band transition (Fig. 2a); a second (wide-band) transition is visible as kink only in high-precision QMC data (circles, crosses) and after adding a linear term (Fig. 2b). Possible signals from this transitions cannot be distinguished from numerical errors in earlier QMC data [5] (squares) since they exceed 100% at both transitions (Fig. 2c).

## 2. Limit of small inter-orbital coupling

Clearly, the resolution of two orbital-selective Mott transitions with critical interactions differing by only about 20% is a very challenging task, in particular at temperatures attainable using QMC. In this situation, much insight can be gained by abandoning the constraint  $U' + 2J = U$  fulfilled in nearly all earlier studies and instead studying the limit of small inter-orbital coupling. Hence, we consider  $H = H_1 + \alpha H_2$  with  $0 \leq \alpha \leq 1$  so that  $\alpha = 0$  corresponds to uncoupled orbitals and  $\alpha = 1$  to the case studied previously.

It is a priori clear, that for  $\alpha = 0$  each orbital should undergo a usual Mott transition at an interaction determined by the corresponding bandwidth ( $W = 2$  for the narrow,  $W = 4$  for the wide band); note however, that even in this case the QMC results for both orbitals have no scaling relation at fixed  $T > 0$ . This is seen in Fig. 3: For  $\alpha = 0$ , a large hysteresis region appears in the wide-band quasiparticle weight (uppermost, grey line) while only a single coex-

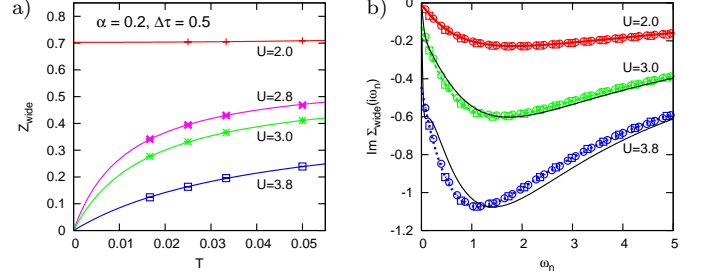


Fig. 4. a) Discrete QMC estimates of wide-band quasiparticle weights for  $\alpha = 0.2$ . In OSM phase ( $2.3 \lesssim U \lesssim 3.9$ ),  $Z_{\text{wide}}$  decays to 0 for  $T \rightarrow 0$ . b) In contrast, the self-energy is practically  $T$ -independent in QMC (squares:  $T = 1/20$ , circles:  $T = 1/40$ ), consistent with DIA for  $T = 0$  (solid lines).

istence point is resolved for the narrow band (at  $T = 1/40$ ). Very importantly, the wide-band transition evidently remains first order at small, but significant inter-orbital coupling ( $\alpha = 0.1, \alpha = 0.2$ ). It may be expected that the first-order range (in  $\alpha$ ) increases at lower temperatures which suggests that the wide-band OSMT might be very weakly first order even at  $\alpha = 1$ . However, the alternative of a quantum phase transition at some critical value  $\alpha = \alpha_c$  is equally interesting and warrants further investigation.

## 3. Nature of orbital-selective Mott phase

As shown above, the (discretely estimated) quasiparticle weight  $Z$  is not well suited for detecting the second OSMT. In fact, it is even misleading in the OSM phase: as seen in Fig. 4a,  $Z_{\text{wide}}$  is nearly constant as a function of  $T$  in the metallic Fermi-liquid phase ( $U = 2.0$ ). However, this observable decays to 0 for  $T \rightarrow 0$  in the OSM phase. Naively, one might conclude that the OSM phase becomes indistinguishable from the insulating phase for  $T = 0$ . However, Fig. 4b proves that this is not the case: the self-energies are practically  $T$ -independent both in the metallic and in the OSM phase [with agreement between QMC results for different  $T$  and self-energy functional theory in dynamical impurity approximation (DIA)]; thus, the  $T$  dependence in  $Z_{\text{wide}}$  is an artifact of the discrete approximation. The non-Fermi-liquid character of the wide band in the OSM phase is clearly seen as the finite limit of  $\text{Im} \Sigma$  for  $\omega \rightarrow i0^+$ .

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## References

- [1] V.I. Anisimov, I.A. Nekrasov, D.E. Kondakov, T.M. Rice, and M. Sigrist, *Eur. Phys. J. B* **25**, 191 (2002).
- [2] S. Nakatsuji, Y. Maeno, *Phys. Rev. Lett.* **84**, 2666 (2000); *Phys. Rev. B* **62**, 6458 (2000).
- [3] C. Knecht, N. Blümer, and P.G.J. van Dongen, *Phys. Rev. B* **72**, 081103(R) (2005); P. G. J. van Dongen, C. Knecht, and N. Blümer, *phys. stat. sol. (b)* **243**, 116 (2006).
- [4] A. Koga, N. Kawakami, T.M. Rice, and M. Sigrist, *Phys. Rev. Lett.* **92**, 216402 (2004).
- [5] A. Liebsch, *Phys. Rev. B* **70**, 165103 (2004).
- [6] A. Koga, N. Kawakami, T. Rice, and M. Sigrist, *Physica B* **359-361**, 1366 (2005).